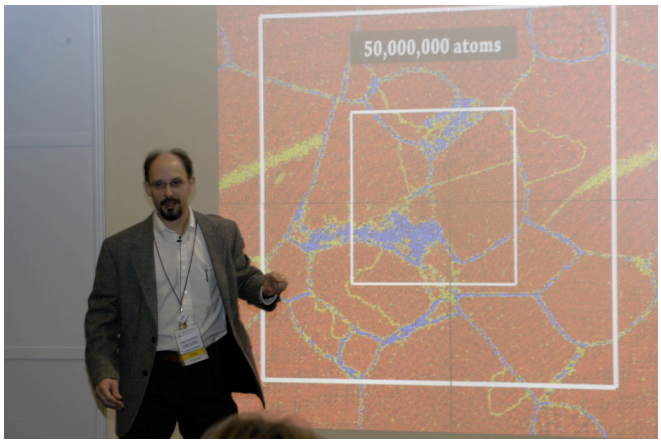
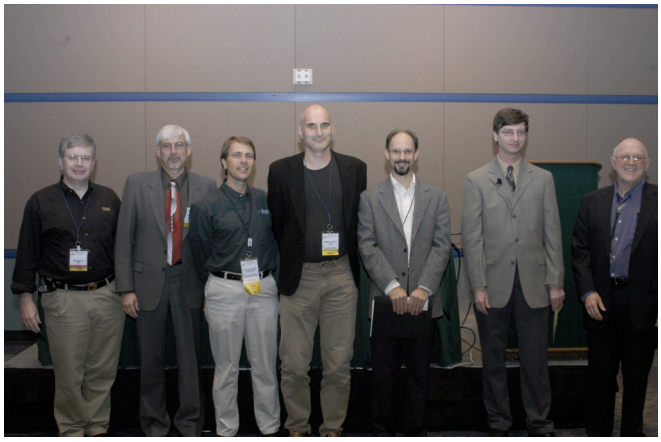
CAR Personnel Help Win Gordon Bell Prize at SC|05

CAR staff members figured prominently on three of the six teams that were finalists for the prestigious Gordon Bell Prize awarded at SC|05 in Seattle. The annual award, which recognizes outstanding achievement in high-performance computing, was presented to an LLNL team headed by Fred Streitz (PAT) for its contribution, *100+ TFlop/s Solidification Simulations on BlueGene/L*.



Fred Streitz (PAT) explains the significant advance in understanding solidification that results from the increased scale of the classical molecular dynamics simulation.

Streitz's team included CASC's Bor Chan, Bronis de Supinski and Kim Yates, as well as PAT's Jim Glosli and Mehul Patel, and IBM's Jim Sexton and John Gunnels. The team investigated solidification in tantalum and uranium systems that ranged in size up to 524,288,000 atoms on LLNL's recently installed IBM BlueGene/L supercomputer. Congratulations!

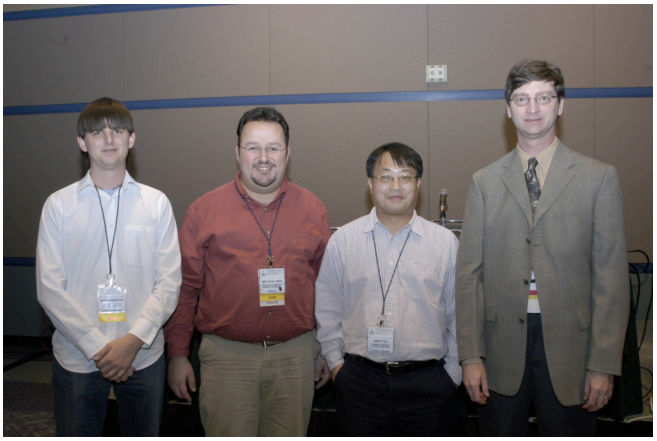


Gordon Bell Award winners (L-R) Jim Sexton (IBM), Kim Yates (CASC), Bronis de Supinski (CASC), Jim Glosli (PAT) and Fred Streitz (PAT), as well as award session chair Bill Gropp (Argonne National Laboratory) and the eponymous Gordon Bell. Not pictured, Bor Chan (CASC) and Mehul Patel (PAT).

A second CAR team, led by Francois Gygi, made it to the final bracket for their contribution, *Large-Scale First-Principles Molecular Dynamics Simulations on the BlueGene/L Platform using the Qbox Code.* The calculations were carried out using the full quantum-mechanical interactions necessary for understanding the details of very complex physical and biological systems. The team achieved a remarkable 64 TFlop/s performance on a problem that was very difficult to parallelize.

Team members (L-R) Kim Yates (CASC), Christoph Ueberhueber (Vienna University of Technology), Franz Franchetti (Carnegie Mellon University), Erik Draeger (CASC), François Gygi, and Bronis de Supinski (CASC), as well as Bill Gropp (ANL). Not pictured, John Gunnels and Jim Sexton (IBM), Stefan Kral, Jeurgen Lorenz, (Vienna University of Technology).

The third CAR team to make it to the final bracket tackled a very different problem and summarized their results in a paper entitled *A Scalable Distributed Parallel Breadth-First Search Algorithm on BlueGene/L.* They devised new algorithms suitable for searching graphs with up to 3 billion vertices and 30 billion edges.



Team members (L-R) Keith Henderson (CASC), Umi Catalyurek (Ohio State University), and Andy Yoo (CASC), with Bill Gropp (ANL). Not pictured, Edmond Chow (DE Shaw Research), and Bill McLendon and Bruce Hendrickson (Sandia National Laboratory)

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